

“Carbon dynamics”
during oxidation and reoxidation of SiC
and
the role of nitrogen -- again

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Theory: S. Wang, S. G. Kim, M. Di Ventra
Microscopy: G. Duscher, S. J. Pennycook (ORNL)
Growth/characterization: L. C. Feldman et al. (Vanderbilt)
J. R. Williams et al. (Auburn)

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Oxidation of SiC

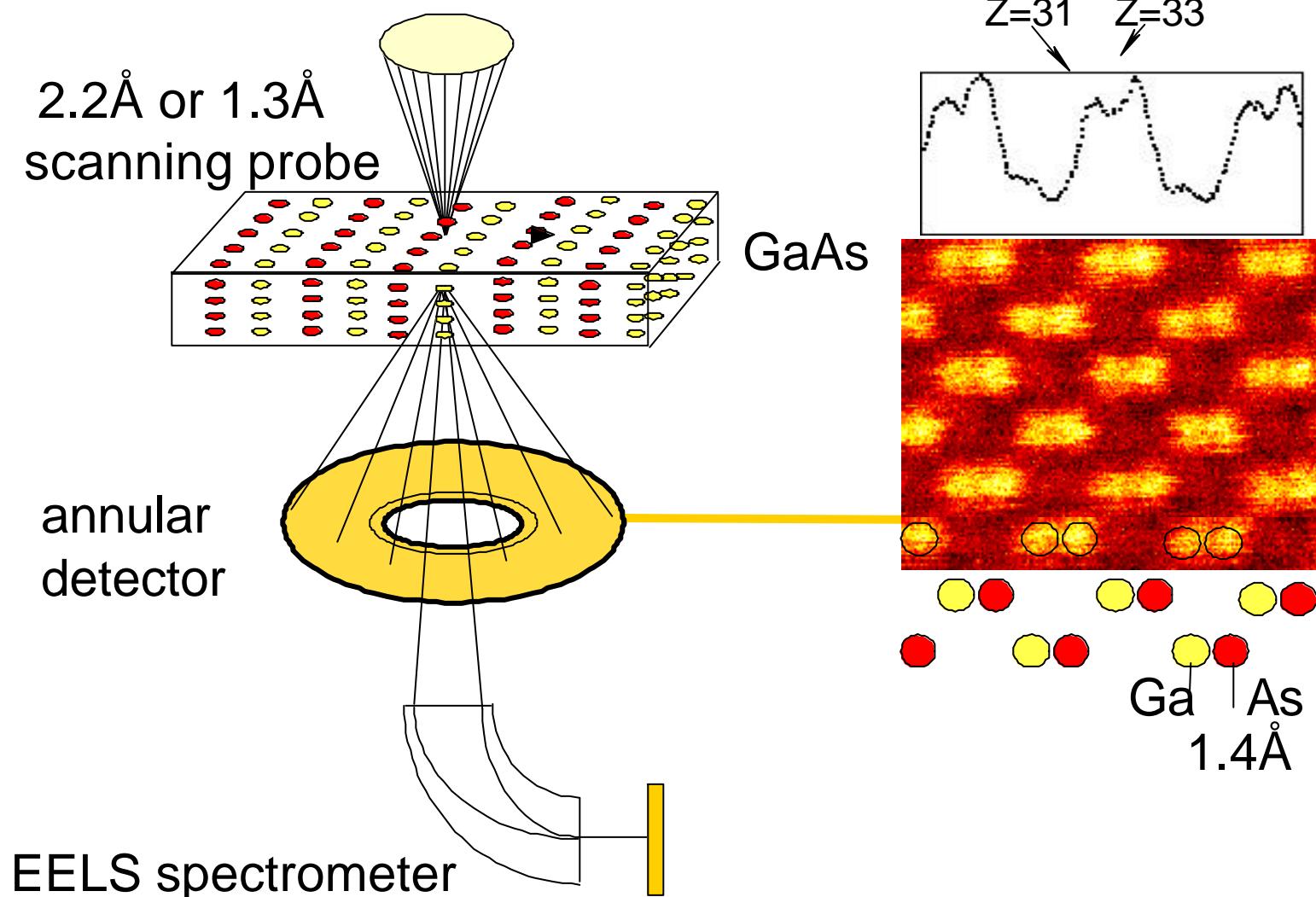
Experiments:

- Step 1: Oxidation at 1100 °C; growth of SiO_2
- Step 2: Reoxidation at 900 °C

Questions:

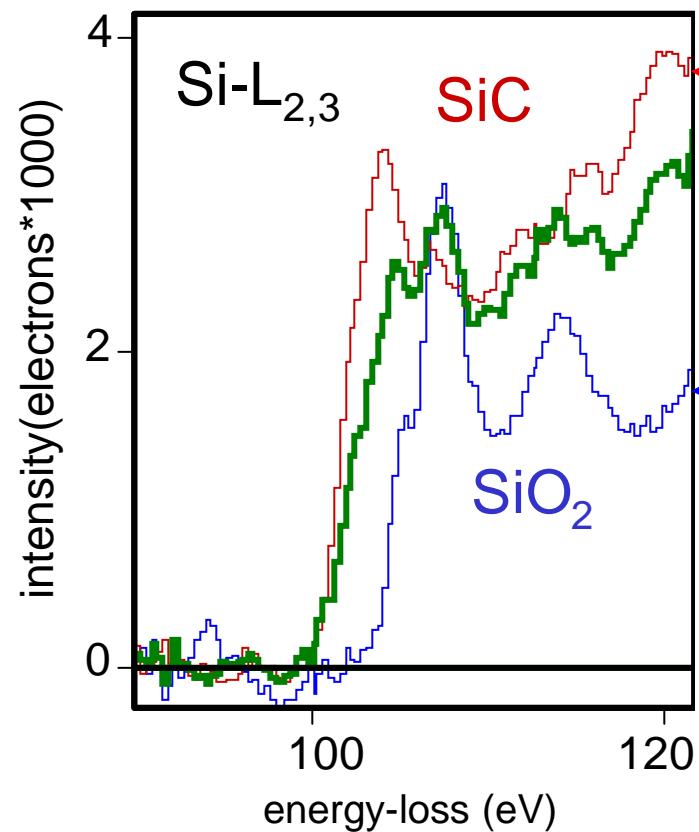
- How is C removed? (Evidence for CO)
- Is C left in SiO_2 or at interface by Step 1?
- What does reoxidation do?

Z-contrast/EELS STEM



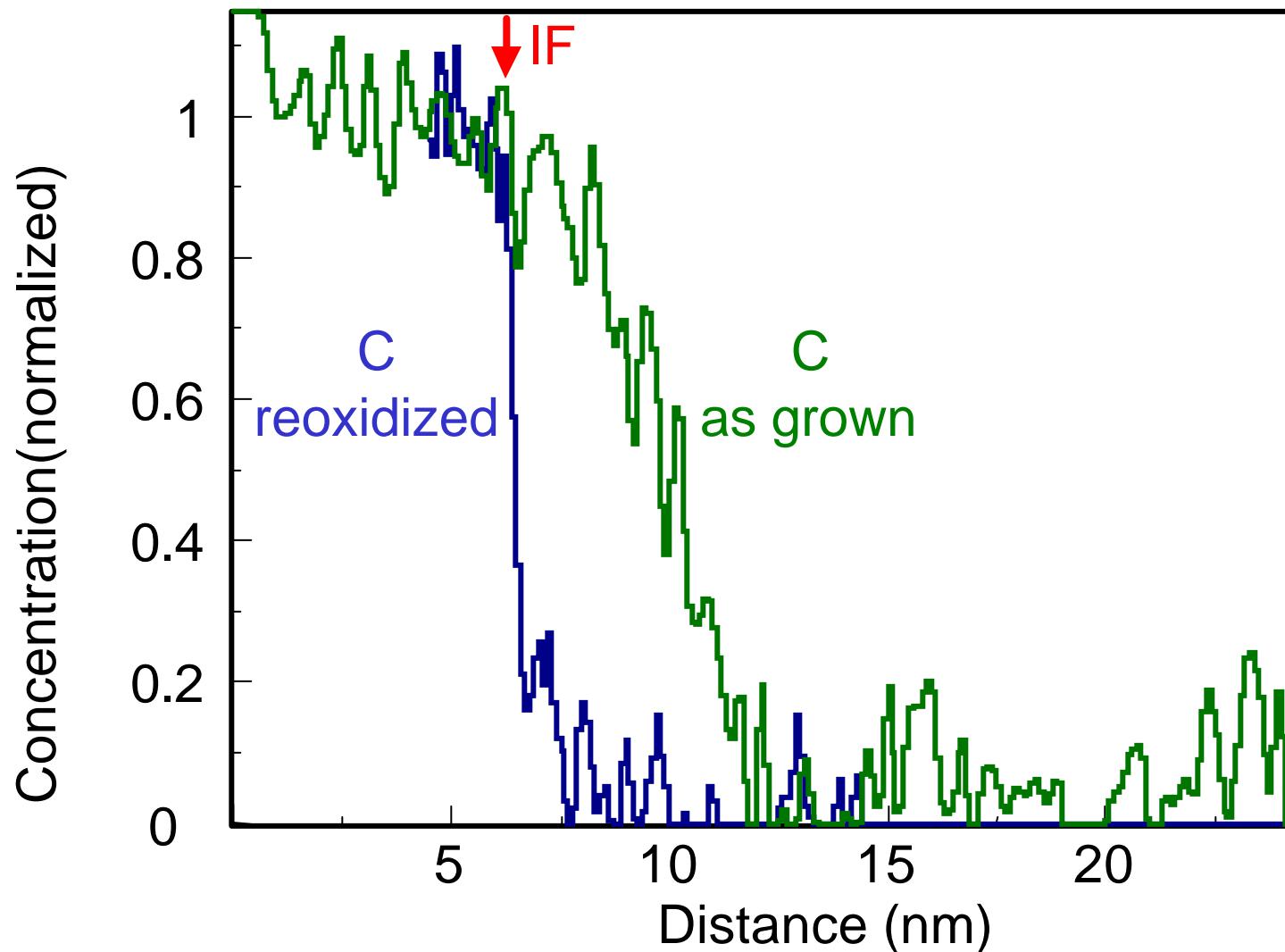
SiC-SiO₂ interface

EELS



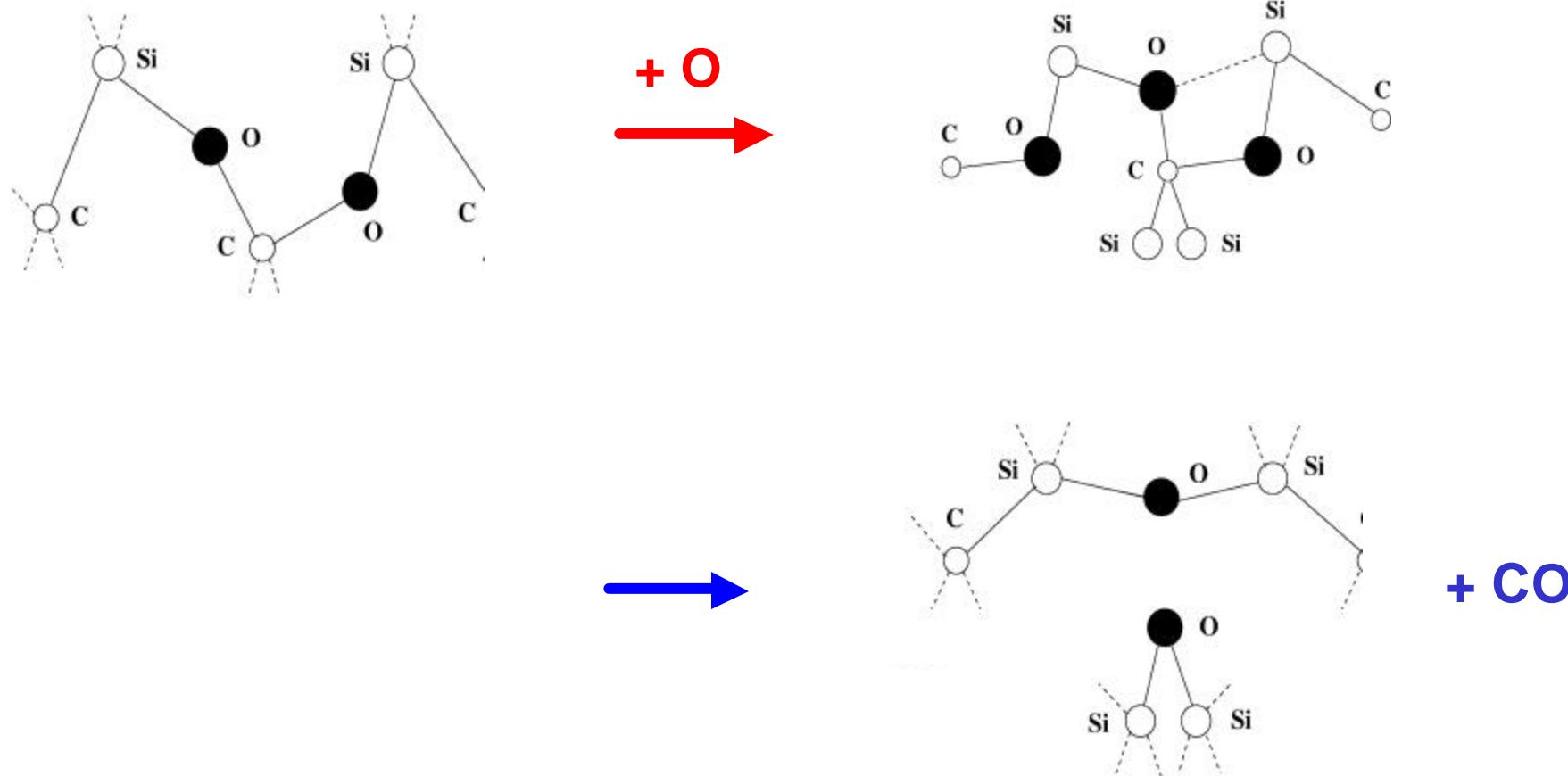
Z-contrast image

Carbon Profile
across as-grown and reoxidized SiC-SiO₂ interfaces

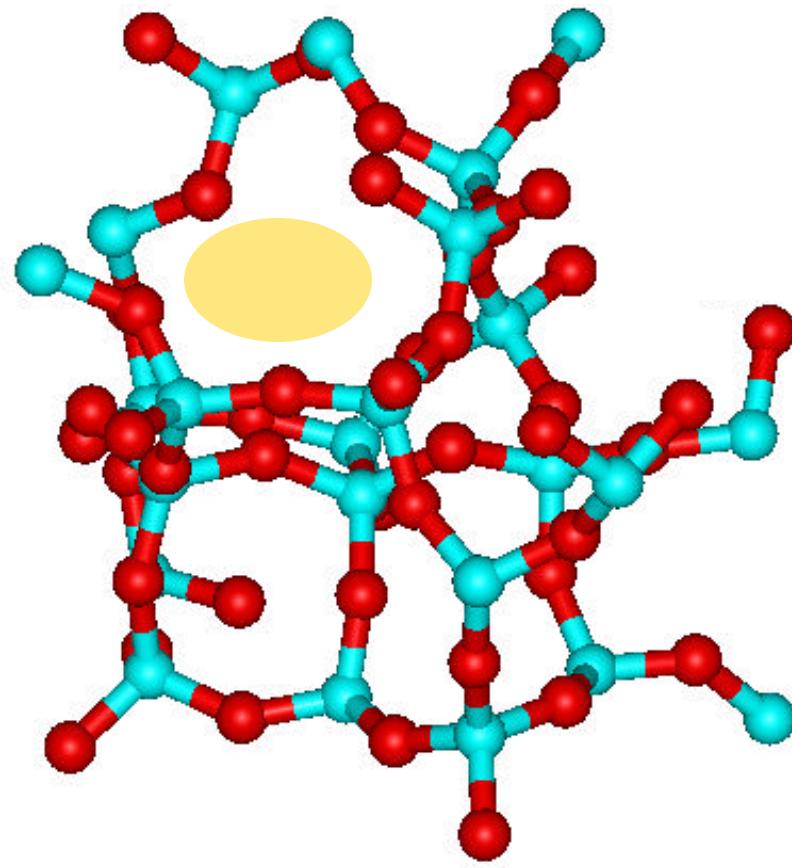


Step 1: Oxidation of SiC

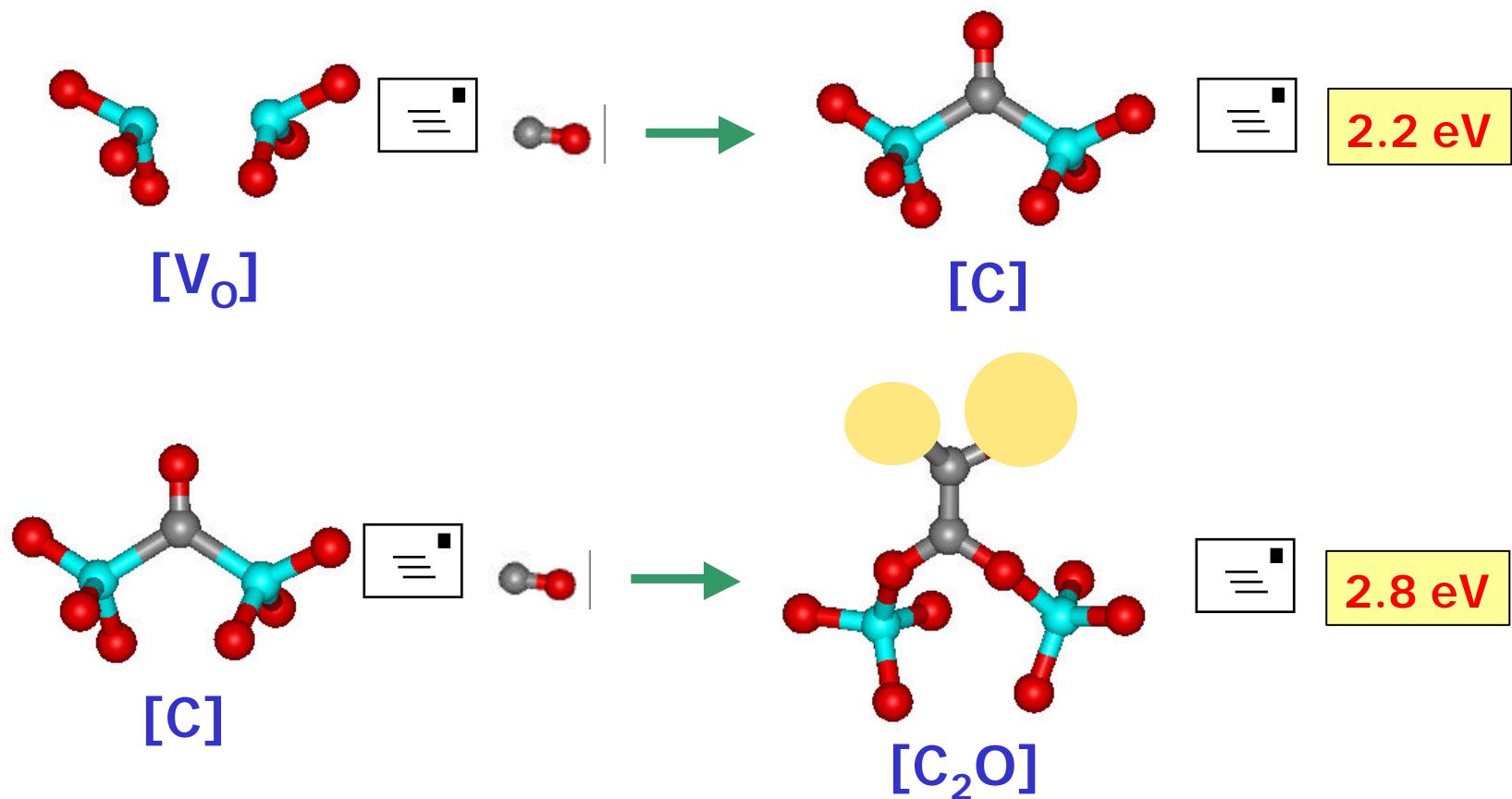
- At the interface: generation of CO



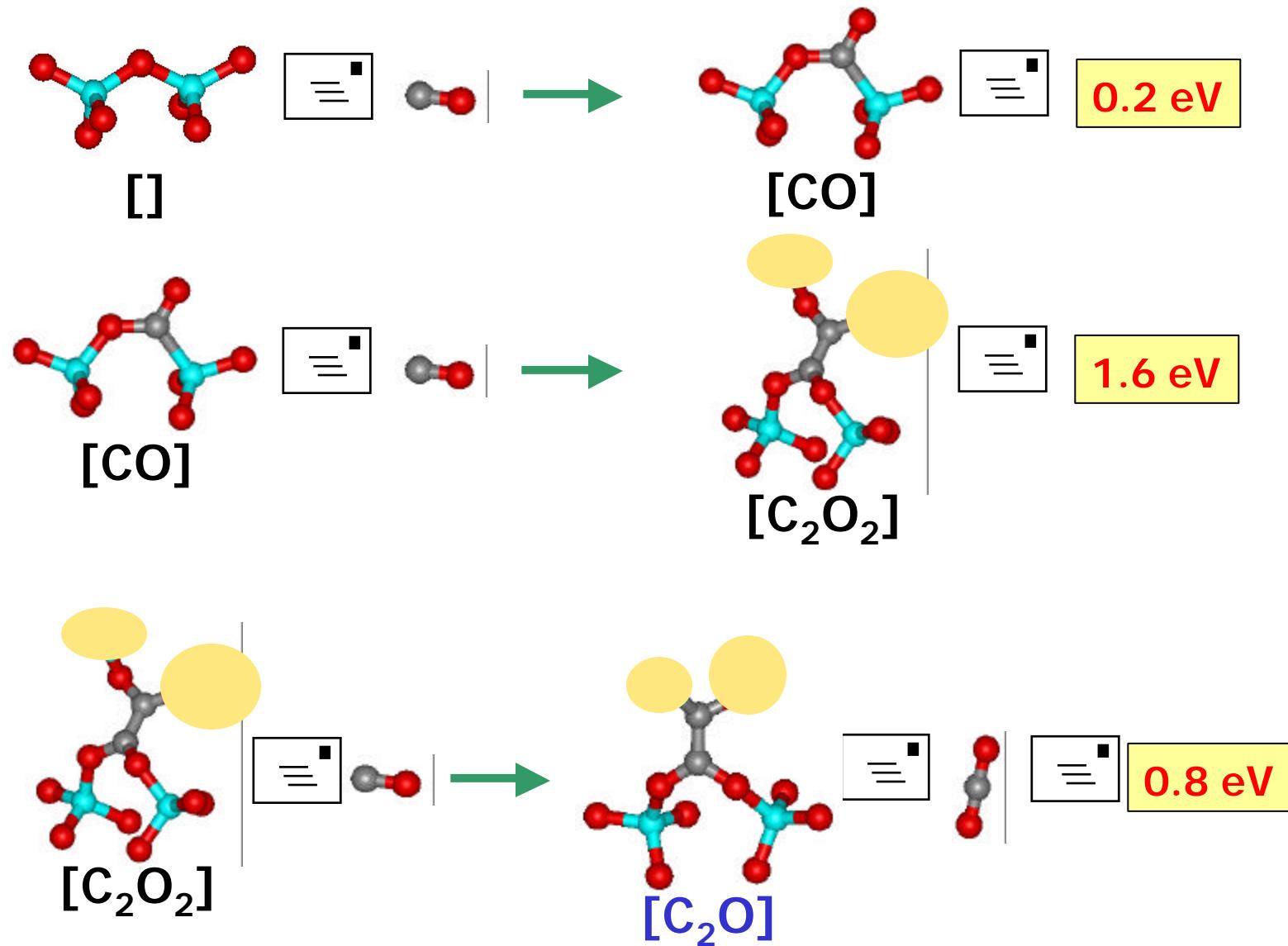
CO in SiO₂



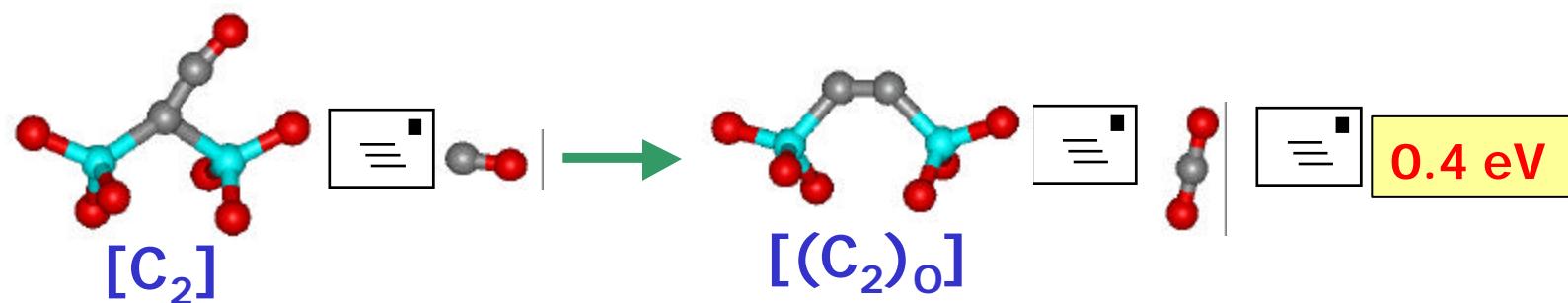
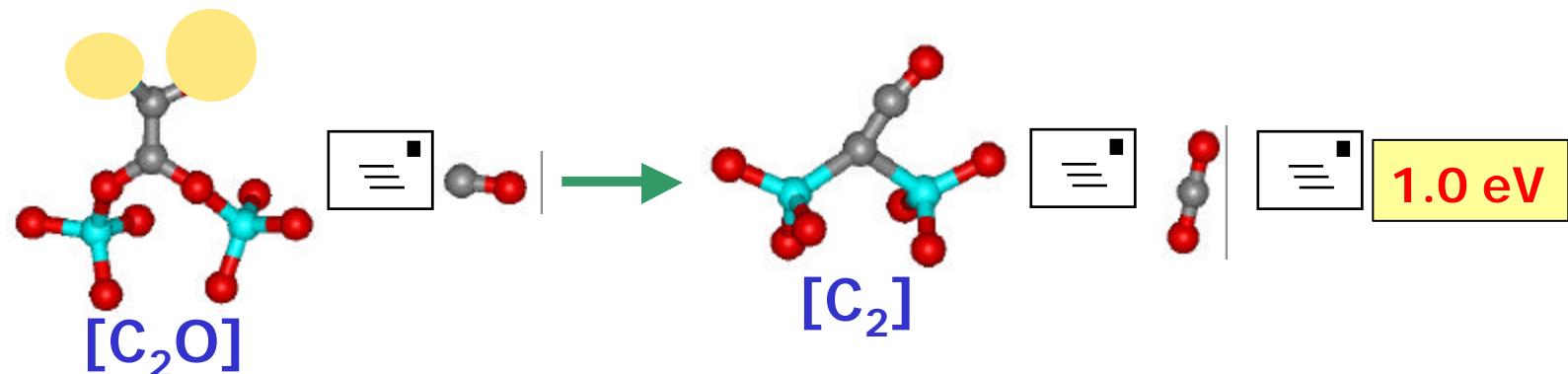
Pre-existing oxygen vacancy



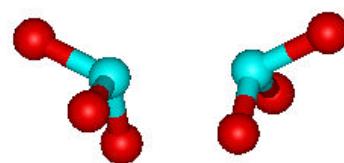
CO in SiO₂ without vacancies



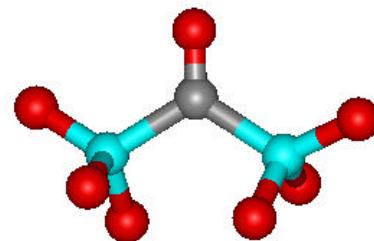
Further reduction of C clusters



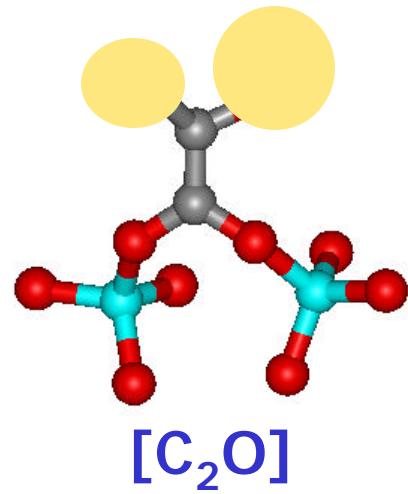
Summary: Oxygen-deficient Defects



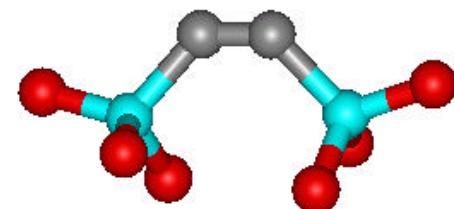
$[V_O]$



$[C]$

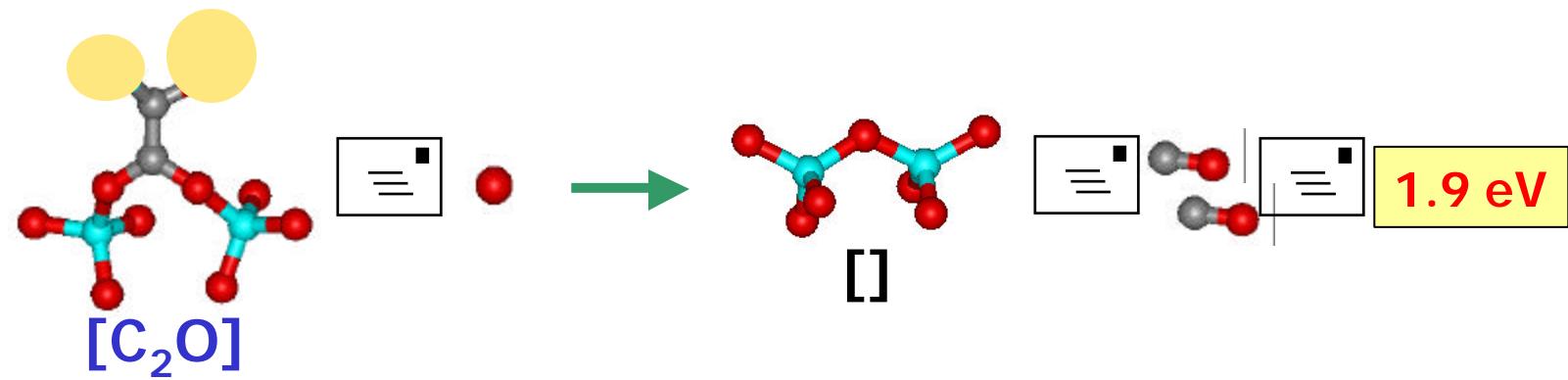
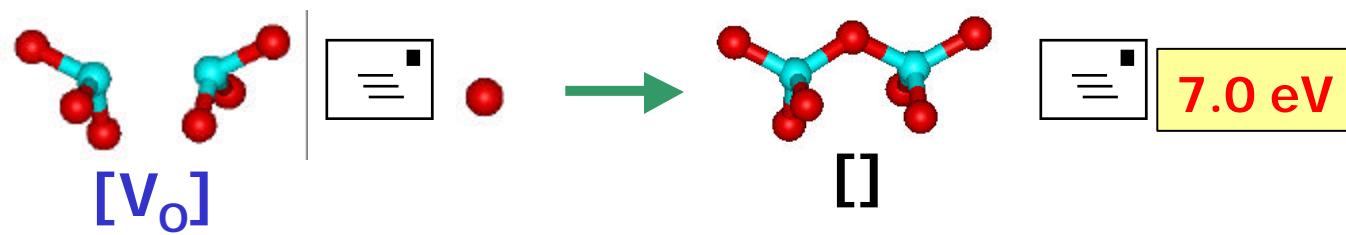


$[C_2]$

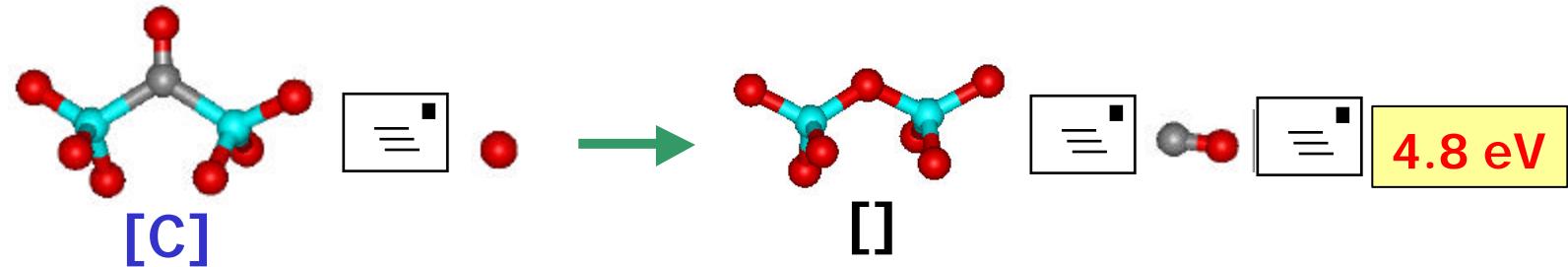
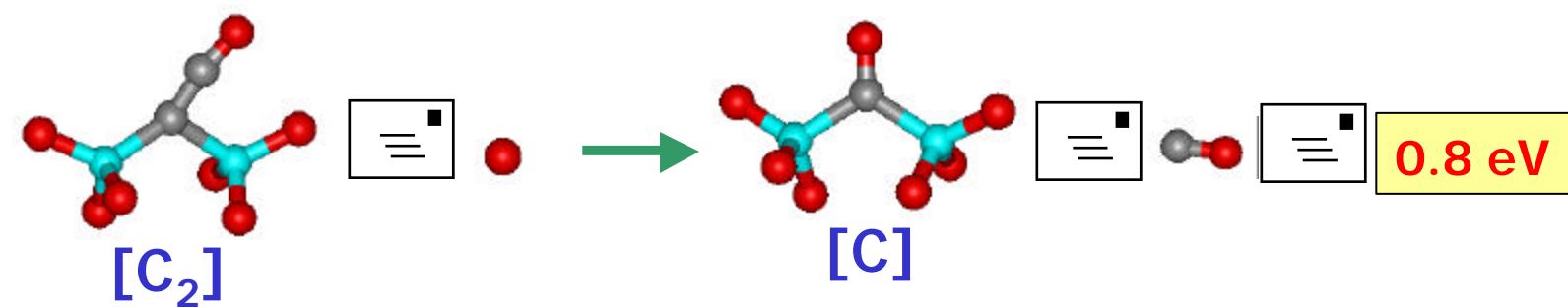
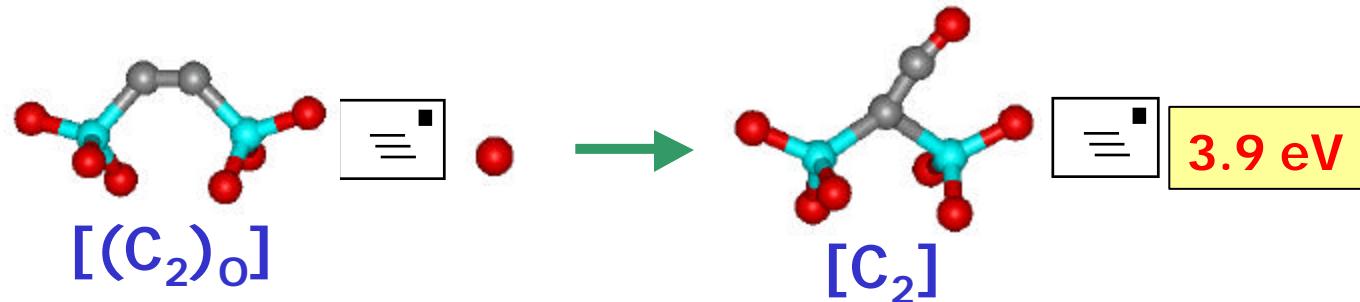


$[(C_2)_o]$

Reoxidation I



Reoxidation II



SUMMARY

Oxidation at 1100 °C

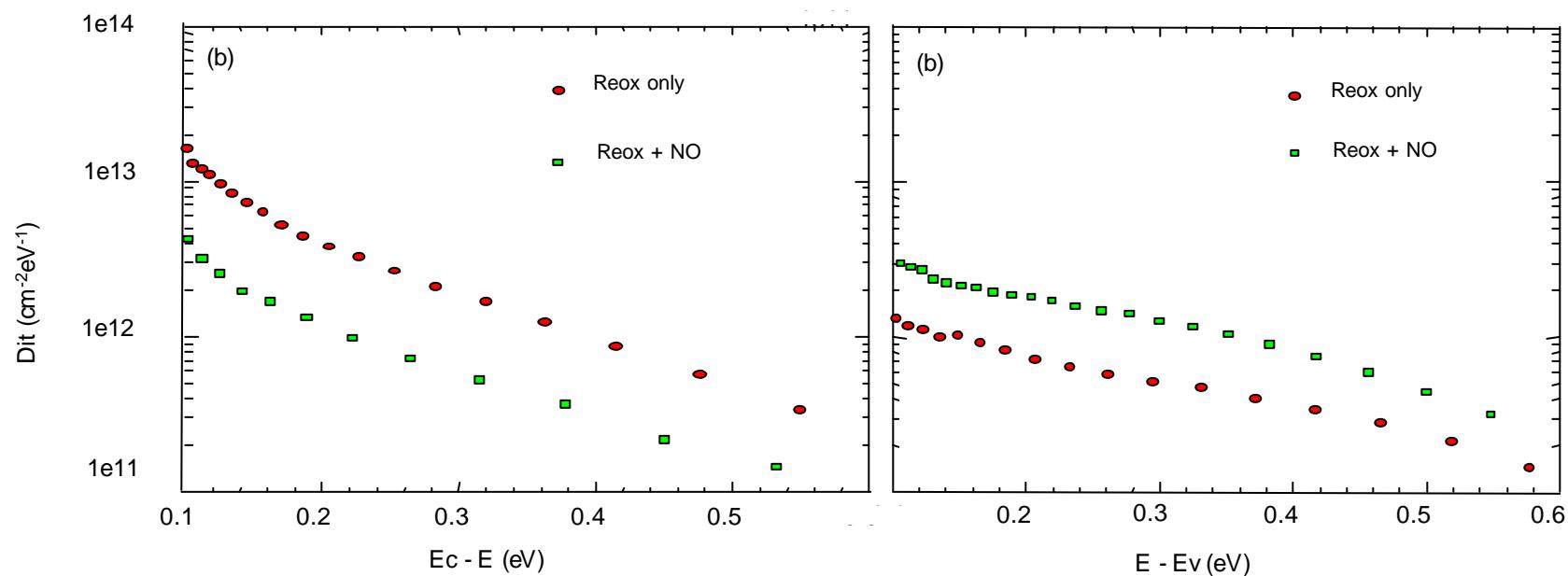
- At the interface: generation of CO
- In the oxide:
 - ▶ CO migrates and gets out
 - ▶ CO forms clusters
 - ▶ Other CO's take up O from CO clusters, leave as CO₂
 - ▶ Net result: O-deficient C clusters

Reoxidation at 900 °C

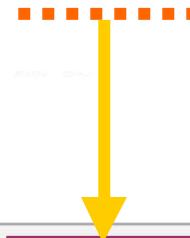
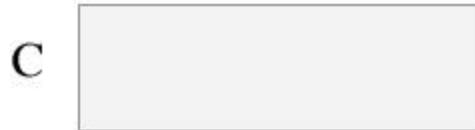
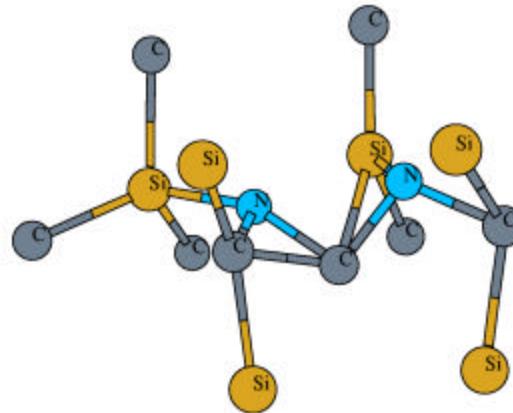
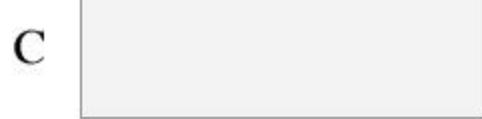
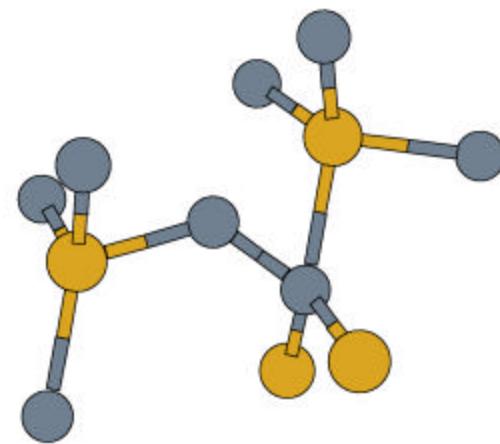
- C clusters dissolve into CO's

NO annealing after reoxidation

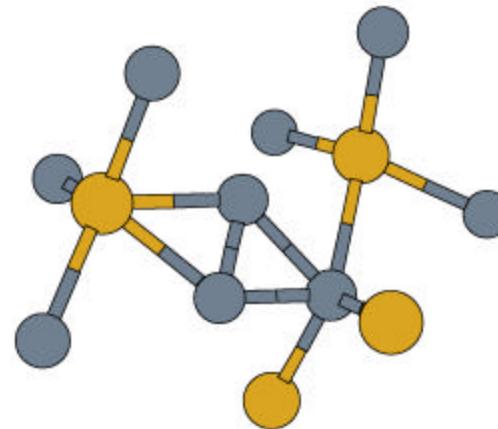
Experiments



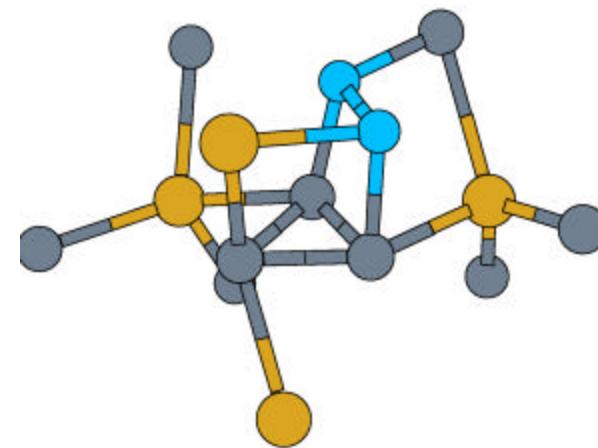
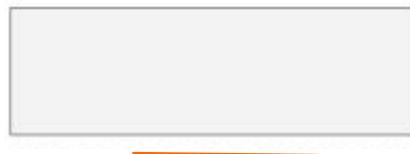
C clusters: 1C



C clusters: 2C



C



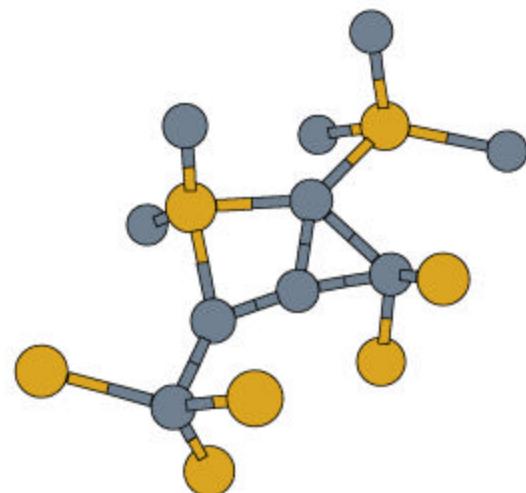
C



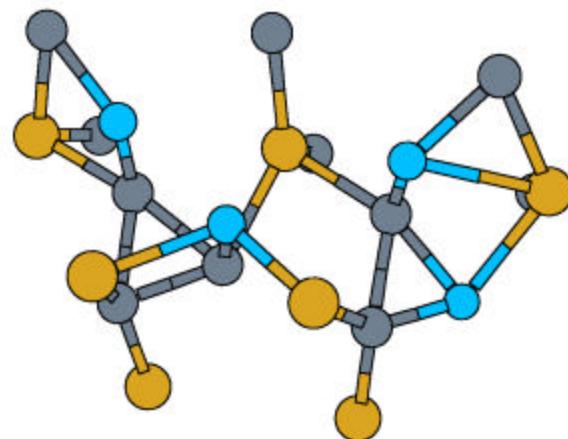
V



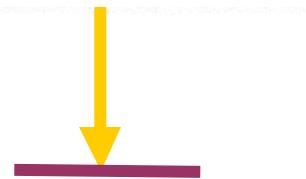
C clusters: 3C



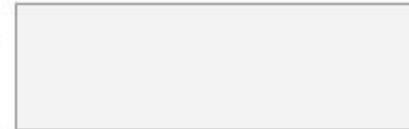
C



C



V



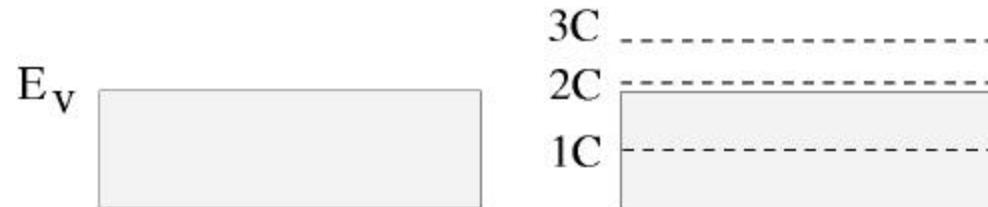
Nitrogen annealing of C clusters: trends



without N

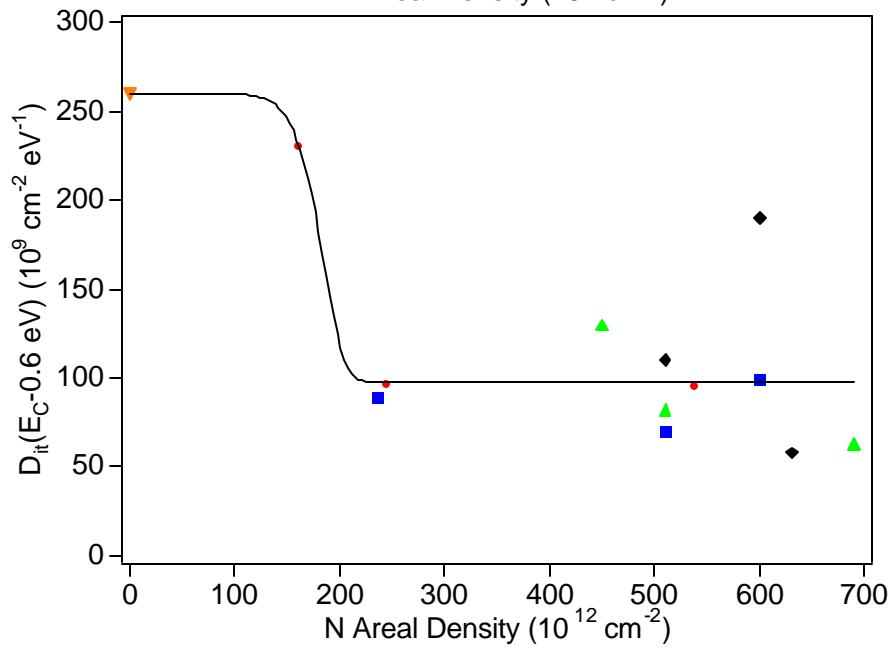
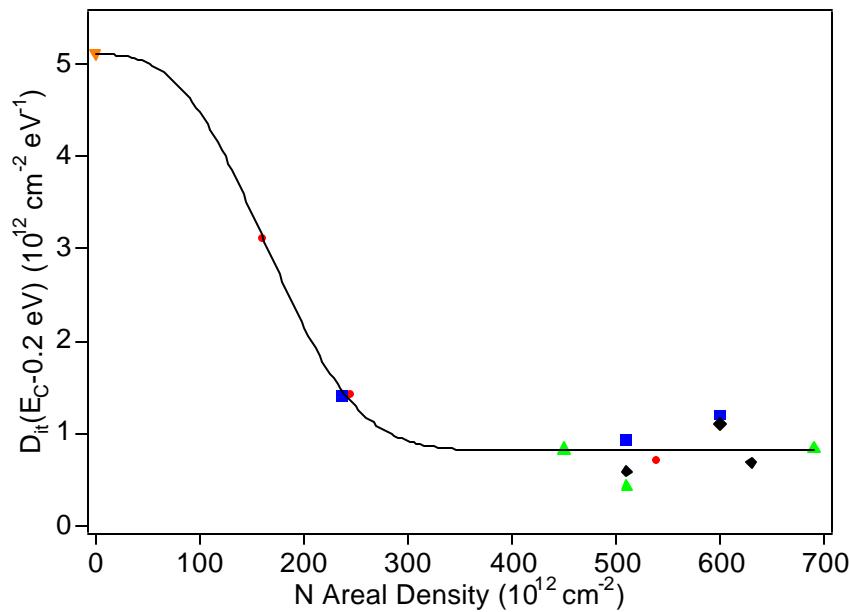


with N



(a)

(b)



Nitrogen passivates 2C and 3C and generates 1C

